Homework 2, Dowling

1. The provided code creates a data frame called "df1", with 3 columns: Name, State and Sales. There are 12 rows of data in the table.

```
> df1
        Name          State Sales
1      James         Alaska    14
2       Paul     California    24
3   Richards          Texas    31
4     Marico North Carolina    12
5   Samantha     California    13
6       Ravi          Texas     7
7      Raghu         Alaska     9
8   Richards          Texas    31
9     George North Carolina    18
10       Ema         Alaska    16
11  Samantha     California    18
12 Catherine          Texas    14
```

The following two commands appear to be different ways to sum Sales by State:

```
> df1 %>% group_by(State) %>% summarise(sum_sales = sum(Sales))
# A tibble: 4 × 2
  State          sum_sales
  <chr>              <dbl>
1 Alaska                39
2 California            55
3 North Carolina        30
4 Texas                 83
```

```
> aggregate(df1$Sales, by=list(df1$State), FUN=sum)
        Group.1  x
1        Alaska 39
2    California 55
3 North Carolina 30
4         Texas 83
```

2. The first few rows (head) of WorldCupMatches look like this (not easy to read in larger font size, so I decreased the size):

```
> library(rstudioapi)
> setwd(dirname(rstudioapi::getActiveDocumentContext()$path))
> wc <- read.csv("../data/WorldCupMatches.csv")
> head(wc)
  Year             Datetime   Stage        Stadium        City Home.Team.Name Home.Team.Goals Away.Team.Goals
1 1930 13 Jul 1930 - 15:00  Group 1        Pocitos Montevideo          France               4               1
2 1930 13 Jul 1930 - 15:00  Group 4 Parque Central Montevideo             USA               3               0
3 1930 14 Jul 1930 - 12:45  Group 2 Parque Central Montevideo      Yugoslavia               2               1
4 1930 14 Jul 1930 - 14:50  Group 3        Pocitos Montevideo         Romania               3               1
5 1930 15 Jul 1930 - 16:00  Group 1 Parque Central Montevideo       Argentina               1               0
6 1930 16 Jul 1930 - 14:45  Group 1 Parque Central Montevideo           Chile               3               0
  Away.Team.Name Win.conditions Attendance Half.time.Home.Goals Half.time.Away.Goals               Referee
1         Mexico                      4444                    3                    0 LOMBARDI Domingo (URU)
2        Belgium                     18346                    2                    0      MACIAS Jose (ARG)
3         Brazil                     24059                    2                    0    TEJADA Anibal (URU)
4           Peru                      2549                    1                    0  WARNKEN Alberto (CHI)
5         France                     23409                    0                    0    REGO Gilberto (BRA)
6         Mexico                      9249                    1                    0  CRISTOPHE Henry (BEL)
              Assistant.1              Assistant.2 RoundID MatchID Home.Team.Initials Away.Team.Initials
1    CRISTOPHE Henry (BEL)       REGO Gilberto (BRA)     201    1096               FRA               MEX
2 MATEUCCI Francisco (URU)     WARNKEN Alberto (CHI)     201    1090               USA               BEL
3  VALLARINO Ricardo (URU)       BALWAY Thomas (FRA)     201    1093               YUG               BRA
```

```
4      LANGENUS Jean (BEL)   MATEUCCI Francisco (URU)     201    1098               ROU               PER
5     SAUCEDO Ulises (BOL) RADULESCU Constantin (ROU)     201    1085               ARG               FRA
6  APHESTEGUY Martin (URU)        LANGENUS Jean (BEL)     201    1095               CHI               MEX
```

a. Rows/cols

```
> nrow(wc)
[1] 852
> ncol(wc)
[1] 20
```

b. Summary

```
> summary(wc)
      Year        Datetime            Stage             Stadium             City           Home.Team.Name
 Min.   :1930   Length:852         Length:852         Length:852         Length:852         Length:852
 1st Qu.:1970   Class :character   Class :character   Class :character   Class :character   Class :character
 Median :1990   Mode  :character   Mode  :character   Mode  :character   Mode  :character   Mode  :character
 Mean   :1985
 3rd Qu.:2002
 Max.   :2014

 Home.Team.Goals  Away.Team.Goals Away.Team.Name     Win.conditions       Attendance     Half.time.Home.Goals
 Min.   : 0.000   Min.   :0.000   Length:852         Length:852         Min.   :  2000   Min.   :0.0000
 1st Qu.: 1.000   1st Qu.:0.000   Class :character   Class :character   1st Qu.: 30000   1st Qu.:0.0000
 Median : 2.000   Median :1.000   Mode  :character   Mode  :character   Median : 41580   Median :0.0000
 Mean   : 1.811   Mean   :1.022                                         Mean   : 45165   Mean   :0.7089
 3rd Qu.: 3.000   3rd Qu.:2.000                                         3rd Qu.: 61374   3rd Qu.:1.0000
 Max.   :10.000   Max.   :7.000                                         Max.   :173850   Max.   :6.0000
                                                                        NA's   :2
 Half.time.Away.Goals   Referee          Assistant.1        Assistant.2          RoundID
 Min.   :0.0000       Length:852         Length:852         Length:852         Min.   :     201
 1st Qu.:0.0000       Class :character   Class :character   Class :character   1st Qu.:     262
 Median :0.0000       Mode  :character   Mode  :character   Mode  :character   Median :     337
 Mean   :0.4284                                                               Mean   :10661773
 3rd Qu.:1.0000                                                               3rd Qu.:  249722
 Max.   :5.0000                                                               Max.   :97410600

    MatchID          Home.Team.Initials Away.Team.Initials
 Min.   :       25   Length:852         Length:852
 1st Qu.:     1189   Class :character   Class :character
 Median :     2191   Mode  :character   Mode  :character
 Mean   : 61346868
 3rd Qu.: 43950059
 Max.   :300186515
```

c. Unique locations

```
> length(unique(wc$City))
[1] 151
```

d. Average attendance

```
> mean(wc$Attendance, na.rm = TRUE)
[1] 45164.8
```

e. Total goals per team

```
> goal <- aggregate(wc$Home.Team.Goals, by=list(wc$Home.Team.Name), FUN=sum)
> colnames(goal) <- c("HomeTeam", "TotalGoals")
> print(head(goal))
   HomeTeam TotalGoals
1   Algeria          5
2    Angola          0
3 Argentina        111
4 Australia          7
5   Austria         31
6   Belgium         27
```

f. Average annual attendees

```
> attend <- aggregate(wc$Attendance, by=list(wc$Year), FUN=mean, na.rm = TRUE)
> colnames(attend) <- c("Year", "AverageAttendance")
> print(head(attend))
  Year AverageAttendance
1 1930          32808.28
2 1934          21352.94
3 1938          20872.22
4 1950          47511.18
5 1954          29561.81
6 1958          23423.14
```

3. Metabolites

```
> mb <- read.csv("../data/metabolite.csv")
> head(mb)
      Label  Phe Pro Ser Thr ADMA alpha.AAA c4.OH.Pro Carnosine Creatinine  DOPA Dopamine Histamine Kynurenine
1 Alzheimer 72.8 166 170 282 1.15     0.760     0.236     1.270       49.9 0.265    0.233     0.225       5.21
2 Alzheimer 93.4 138 142 217 1.05     0.929     0.189     1.350       48.8 0.252       NA     0.211       5.44
3 Alzheimer 68.6 161 158 208 1.00     0.620     0.198     0.998       30.4 0.268       NA     0.217       5.20
4 Alzheimer 94.1 129 162 201 1.10     0.795        NA     0.675       80.1 0.264    0.234     0.209       5.80
5 Alzheimer 79.8 126 115 199 1.24     1.360        NA     1.280       60.5 0.271    0.231     0.210       4.46
  Met.SO Nitro.Tyr PEA Putrescine Sarcosine Serotonin Spermidine Spermine t4.OH.Pro Taurine SDMA   C0   C10
1  0.526     0.027  NA      0.068      17.8     0.147      0.188       NA      24.0     125 1.13 18.2 0.059
2  0.387        NA  NA      0.087      20.2     0.231      0.233       NA      29.3     120 1.65 17.0 0.051
3  0.651        NA  NA      0.260      14.4     0.196      0.384       NA      20.9     139 1.57 12.6 0.083
4  0.389        NA  NA      0.110      18.7     0.255      0.353       NA      23.1     159 1.34 23.5 0.071
5  0.466        NA  NA      0.118      22.5     0.390      0.473       NA      26.9     149 1.24 13.6 0.139
  C10.1 C10.2   C12 C12.DC C12.1   C14 C14.1 C14.1.OH C14.2 C14.2.OH   C16 C16.OH C16.1 C16.1.OH C16.2
1 0.312 0.038 0.030  0.042 0.290 0.023 0.019    0.008 0.008    0.006 0.046  0.008 0.009    0.007 0.005
2 0.288 0.039 0.038  0.038 0.265 0.026 0.017    0.008 0.009    0.009 0.070  0.009 0.013    0.006 0.006
3 0.357 0.054 0.032  0.048 0.302 0.021 0.031    0.010 0.010    0.009 0.076  0.011 0.019    0.010 0.005
4 0.317 0.040 0.045  0.048 0.275 0.026 0.028    0.010 0.013    0.011 0.074  0.011 0.015    0.008 0.006
5 0.472 0.074 0.056  0.079 0.394 0.034 0.043    0.016 0.025    0.017 0.062     NA 0.024    0.014 0.012
  C16.2.OH   C18 C18.1 C18.1.OH C18.2   C2    C3 C3.OH  C3.1    C4 C3.DC..C4.OH.  C4.1    C5 C5.M.DC
1    0.013 0.013 0.024    0.003 0.016 1.97 0.354 0.008 0.015 0.082         0.045 0.025 0.094   0.023
2    0.012 0.014 0.025    0.003 0.028 1.95 0.184 0.009 0.013 0.108         0.080 0.025 0.077   0.032
3    0.013 0.016 0.025       NA 0.018 1.70 0.371    NA 0.012 0.057         0.035 0.039 0.096   0.045
4    0.009 0.020 0.035    0.004 0.033 2.10 0.278 0.010 0.017 0.110         0.077 0.031 0.145   0.034
5    0.025 0.031 0.034    0.012 0.017 5.62 0.436 0.029 0.035 0.106         0.099 0.069 0.141   0.094
  C5.OH..C3.DC.M.  C5.1 C5.1.DC C6..C4.1.DC. C5.DC..C6.OH.  C6.1 C7.DC    C8    C9 lysoPC.a.C14.0
1           0.026 0.030   0.020        0.022         0.014 0.018 0.011 0.062 0.016           2.23
2           0.026 0.024   0.021        0.030         0.018 0.015 0.010 0.058 0.014           1.97
3           0.024 0.037   0.018        0.022         0.029 0.031 0.021 0.090 0.017           2.12
4           0.041 0.035   0.016        0.029         0.016 0.027 0.017 0.091 0.018           2.19
5           0.058 0.073   0.049        0.052         0.040 0.040 0.036 0.192 0.041           1.88
  lysoPC.a.C16.0 lysoPC.a.C16.1 lysoPC.a.C17.0 lysoPC.a.C18.0 lysoPC.a.C18.1 lysoPC.a.C18.2 lysoPC.a.C20.3
1           37.9           2.66          0.446           9.00           8.58           7.27          1.830
2           22.1           1.31          0.270           5.35           3.94           4.42          0.958
3           33.7           2.53          0.399           7.51           7.73           8.02          2.050
4           32.8           2.39          0.323           7.21           7.22           7.62          1.640
5           24.5           1.27          0.382           6.66           5.39           3.60          0.970
  lysoPC.a.C20.4 lysoPC.a.C24.0 lysoPC.a.C26.0 lysoPC.a.C26.1 lysoPC.a.C28.0 lysoPC.a.C28.1 PC.aa.C24.0
1           8.25          0.079          0.113          0.053          0.108          0.072       0.082
2           4.60          0.059          0.066          0.042          0.076          0.058       0.065
3           9.84          0.075          0.126          0.049          0.078          0.092       0.099
4           6.75          0.066          0.086          0.045          0.076          0.076       0.076
5           6.26          0.084          0.118          0.053          0.092          0.072       0.069
  PC.aa.C26.0 PC.aa.C28.1 PC.aa.C30.0 PC.aa.C32.0 PC.aa.C32.1 PC.aa.C32.2 PC.aa.C32.3 PC.aa.C34.1 PC.aa.C34.2
1       0.438       0.571        2.35        11.4        9.22          NA       0.092       109.0        71.0
2       0.409       0.521        1.99        12.7        5.40          NA       0.067        64.2        60.5
3       0.458       0.605        2.69        16.6       11.60          NA       0.105       108.0        83.1
4       0.486       0.685        3.33        18.6       13.30       0.053       0.079       106.0        93.6
5       0.401       0.513        1.78        13.8        5.03          NA       0.102        83.4        35.9
  PC.aa.C34.3 PC.aa.C34.4 PC.aa.C36.0 PC.aa.C36.1 PC.aa.C36.2 PC.aa.C36.3 PC.aa.C36.4 PC.aa.C36.5 PC.aa.C36.6
1       1.430       0.200        2.38        21.7        42.4        42.7       120.0        1.86       0.084
2       0.879       0.127        2.05        14.3        35.6        24.3        83.7        1.05       0.046
```

```
3       1.930       0.210        2.30        19.9        44.9        43.9       146.0        2.09       0.057
4       1.590       0.190        2.57        20.9        48.8        41.2       122.0        1.76       0.070
5       0.709       0.135        1.83        20.5        28.5        21.9        98.1        1.70       0.048
  PC.aa.C38.0 PC.aa.C38.3 PC.aa.C38.4 PC.aa.C38.5 PC.aa.C38.6 PC.aa.C40.1 PC.aa.C40.2 PC.aa.C40.3 PC.aa.C40.4
1       1.230        32.1        95.1       16.80        41.6       0.195       0.074       0.491        3.48
2       0.946        21.9        78.9        9.91        25.1       0.211       0.057       0.358        3.39
3       1.210        34.5       107.0       17.50        36.6       0.212       0.118       0.395        3.56
4       1.160        28.7        92.7       14.30        29.9       0.220       0.097       0.433        3.59
5       1.100        23.3       101.0       13.80        36.2       0.165       0.044       0.525        3.37
  PC.aa.C40.5 PC.aa.C40.6 PC.aa.C42.0 PC.aa.C42.1 PC.aa.C42.2 PC.aa.C42.4 PC.aa.C42.5 PC.aa.C42.6 PC.ae.C30.0
1        5.66        21.8       0.364       0.226       0.108       0.272       0.272       0.291       0.173
2        4.08        14.2       0.419       0.216       0.109       0.336       0.317       0.248       0.147
3        5.34        16.7       0.476       0.281       0.118       0.300       0.206       0.267       0.209
4        5.06        14.0       0.427       0.223       0.119       0.268       0.267       0.254       0.223
5        5.29        22.5       0.125       0.095       0.083       0.206       0.205       0.280       0.095
  PC.ae.C30.1 PC.ae.C30.2 PC.ae.C32.1 PC.ae.C32.2 PC.ae.C34.0 PC.ae.C34.1 PC.ae.C34.2 PC.ae.C34.3 PC.ae.C36.0
1       0.027       0.022        1.65       0.371       0.880        3.66        2.48       0.813       0.498
2       0.024       0.020        2.01       0.360       0.763        2.68        2.32       0.905       0.398
3       0.046       0.030        2.40       0.477       0.938        4.04        2.95       1.030       0.554
4       0.049       0.023        2.47       0.459       0.964        4.06        3.09       1.020       0.552
5       0.082       0.023        1.72       0.316       1.060        3.28        1.70       0.722       0.553
  PC.ae.C36.1 PC.ae.C36.2 PC.ae.C36.3 PC.ae.C36.4 PC.ae.C36.5 PC.ae.C38.0 PC.ae.C38.1 PC.ae.C38.2 PC.ae.C38.3
1        5.64        1.90       1.170        6.96        4.79       0.474       0.287       0.538        2.66
2        3.89        1.54       0.873        6.40        5.36       0.325          NA       0.127        1.80
3        5.95        2.29       1.240        9.05        6.63       0.478       0.285       0.154        2.87
4        4.75        2.01       1.350        8.36        5.97       0.397       0.022       0.144        1.97
5        5.95        1.47       0.760        4.78        4.00       0.430       0.271       0.246        1.80
  PC.ae.C38.4 PC.ae.C38.5 PC.ae.C38.6 PC.ae.C40.1 PC.ae.C40.2 PC.ae.C40.3 PC.ae.C40.4 PC.ae.C40.5 PC.ae.C40.6
1        6.33        5.51        1.95       0.574       0.575       0.940        1.76        1.77        1.59
2        5.37        4.49        1.63       0.281       0.491       0.702        1.43        1.55        1.20
3        7.06        5.64        1.98       0.759       0.654       0.817        1.51        1.64        1.49
4        5.99        5.63        1.97       0.425       0.540       0.742        1.45        1.62        1.25
5        5.45        4.34        1.51       0.430       0.432       0.632        1.10        1.25        1.47
  PC.ae.C42.0 PC.ae.C42.1 PC.ae.C42.2 PC.ae.C42.3 PC.ae.C42.4 PC.ae.C42.5 PC.ae.C44.3 PC.ae.C44.4 PC.ae.C44.5
1       0.629       0.316       0.192       0.277       0.264       0.888       0.065       0.168       0.536
2       0.616       0.260       0.157       0.200       0.311       0.840       0.071       0.220       0.470
3       0.686       0.356       0.241       0.288       0.319       0.957       0.065       0.228       0.565
4       0.637       0.299       0.159       0.208       0.392       0.863       0.069       0.237       0.517
5       0.660       0.355       0.138       0.174       0.162       0.513       0.081       0.154       0.178
  PC.ae.C44.6 SM..OH..C14.1 SM..OH..C16.1 SM..OH..C22.1 SM..OH..C22.2 SM..OH..C24.1 SM.C16.0 SM.C16.1 SM.C18.0
1       0.494         1.420          1.33          2.07          1.86         0.597     44.9     7.99     14.5
2       0.515         1.390          1.25          2.47          2.20         0.640     42.1     6.88     12.7
3       0.603         1.840          1.58          2.69          2.63         0.665     44.8     8.91     14.6
4       0.611         1.720          1.48          2.97          2.84         0.682     52.4     8.61     17.2
5       0.134         0.987          1.48          1.96          1.74         0.478     40.6     5.86     13.0
  SM.C18.1 SM.C20.2 SM.C24.0 SM.C24.1 SM.C26.0 SM.C26.1 H1_1   H1 Urea_N L.Arginine_N L.Leucine_N EDTAca_N
1    10.40    0.290    12.20     27.3    0.147    0.337 3356 3356     NA          NA          NA       NA
2     8.52    0.211    10.40     25.6    0.130    0.317 2509 2509  201.9        22.5        35.3      2.0
3    11.60    0.304    11.50     28.8    0.163    0.364 2661 2661  193.3        21.0        25.4      1.8
4    11.50    0.261    11.80     27.9    0.138    0.353 2652 2652  500.8        16.0        27.1      2.5
5     8.34    0.196     9.29     20.5    0.111    0.283 2258 2258  132.5        13.2        57.9      2.5
  X2.Hydroxybutyrate X3.Hydroxybutyrate Acetate Acetoacetate Acetone Betaine Carnitine Choline Creatine
1                 NA                 NA      NA           NA      NA      NA        NA      NA       NA
2              12.40                8.5    13.2          5.7     5.1    22.0       8.7    14.2     14.5
3              11.33               11.7     5.8          9.3     5.6    19.1      15.3    14.5     17.8
4              12.70                7.2     9.8          4.8     4.0    13.9       7.7    11.8     14.7
5              35.20               44.7    20.2         18.9    18.9    33.9      18.5    27.7     35.4
  Dimethyl.sulfone Ethanol Formate Glucose Glycerol Hypoxanthine Isobutyrate Isopropanol Lactate Malonate
1               NA      NA      NA      NA       NA           NA          NA          NA      NA       NA
2              4.7    16.6    24.6  1489.7    324.6          6.3         3.6         1.9  1171.6     10.4
3              2.1     8.1    27.4  1343.9    201.3          6.0         2.5         2.5  1938.1     13.1
4              1.3     6.4    14.4   629.5    322.0          8.6         2.5         4.4  1037.7      7.6
5              5.5    13.0    40.0  1618.0    271.6          0.0         6.1        11.2  2199.9     11.7
 [ reached 'max' / getOption("max.print") -- omitted 1 rows ]
```

a. Alzheimer's patients

```
> sum(mb$Label == "Alzheimer")
[1] 35
```

b. Missing values per column

```
> head(colSums(is.na(mb)))
Label   Phe   Pro   Ser   Thr  ADMA
    0     0     0     0     0     0
```

c. New data frame with rows missing **Dopamine** value

```
> head(mb1 <- mb[!is.na(mb$Dopamine),])
      Label  Phe Pro Ser Thr ADMA alpha.AAA c4.OH.Pro Carnosine Creatinine  DOPA Dopamine Histamine Kynurenine
1 Alzheimer 72.8 166 170 282 1.15     0.760     0.236     1.270       49.9 0.265    0.233     0.225       5.21
4 Alzheimer 94.1 129 162 201 1.10     0.795        NA     0.675       80.1 0.264    0.234     0.209       5.80
5 Alzheimer 79.8 126 115 199 1.24     1.360        NA     1.280       60.5 0.271    0.231     0.210       4.46
8   Healthy 83.6 119 135 268 1.18     0.779     0.215     0.647       30.6 0.275    0.244     0.214       5.66
9   Healthy 73.7 124 145 307 1.17     0.785     0.186     0.590       39.8 0.259    0.233     0.210       6.36
  Met.SO Nitro.Tyr PEA Putrescine Sarcosine Serotonin Spermidine Spermine t4.OH.Pro Taurine SDMA   C0   C10
1  0.526     0.027  NA       0.068      17.8     0.147      0.188       NA      24.0     125 1.13 18.2 0.059
4  0.389        NA  NA       0.110      18.7     0.255      0.353       NA      23.1     159 1.34 23.5 0.071
5  0.466        NA  NA       0.118      22.5     0.390      0.473       NA      26.9     149 1.24 13.6 0.139
8  0.245     0.002  NA       0.161      23.3     0.215      0.276       NA      10.7     133 1.04 13.3 0.051
9  0.413        NA  NA       0.121      22.1     0.166      0.327       NA      16.0     215 1.24 15.8 0.061
  C10.1 C10.2   C12 C12.DC C12.1   C14 C14.1 C14.1.OH C14.2 C14.2.OH   C16 C16.OH C16.1 C16.1.OH C16.2
1 0.312 0.038 0.030  0.042 0.290 0.023 0.019    0.008 0.008    0.006 0.046  0.008 0.009    0.007 0.005
4 0.317 0.040 0.045  0.048 0.275 0.026 0.028    0.010 0.013    0.011 0.074  0.011 0.015    0.008 0.006
5 0.472 0.074 0.056  0.079 0.394 0.034 0.043    0.016 0.025    0.017 0.062     NA 0.024    0.014 0.012
8 0.217 0.030 0.041  0.035 0.174 0.024 0.017    0.007 0.006    0.007 0.060  0.006 0.010    0.005 0.004
9 0.258 0.036 0.037  0.038 0.228 0.022 0.018    0.007 0.007    0.007 0.054  0.005 0.012    0.005 0.005
  C16.2.OH   C18 C18.1 C18.1.OH C18.2   C2    C3 C3.OH  C3.1    C4 C3.DC..C4.OH.  C4.1    C5 C5.M.DC
1    0.013 0.013 0.024    0.003 0.016 1.97 0.354 0.008 0.015 0.082         0.045 0.025 0.094   0.023
4    0.009 0.020 0.035    0.004 0.033 2.10 0.278 0.010 0.017 0.110         0.077 0.031 0.145   0.034
5    0.025 0.031 0.034    0.012 0.017 5.62 0.436 0.029 0.035 0.106         0.099 0.069 0.141   0.094
8    0.008 0.020 0.025    0.004 0.019 1.66 0.258 0.008 0.012 0.082         0.047 0.021 0.107   0.023
9    0.009 0.014 0.026    0.003 0.016 2.21 0.233 0.008 0.014 0.088         0.029 0.024 0.127   0.024
  C5.OH..C3.DC.M.  C5.1 C5.1.DC C6..C4.1.DC. C5.DC..C6.OH.  C6.1 C7.DC    C8    C9 lysoPC.a.C14.0
1           0.026 0.030   0.020        0.022         0.014 0.018 0.011 0.062 0.016           2.23
4           0.041 0.035   0.016        0.029         0.016 0.027 0.017 0.091 0.018           2.19
5           0.058 0.073   0.049        0.052         0.040 0.040 0.036 0.192 0.041           1.88
8           0.023 0.021   0.017        0.036         0.011    NA 0.009 0.062 0.011           2.13
9           0.024 0.025   0.016        0.026         0.018 0.015 0.013 0.064 0.014           2.10
  lysoPC.a.C16.0 lysoPC.a.C16.1 lysoPC.a.C17.0 lysoPC.a.C18.0 lysoPC.a.C18.1 lysoPC.a.C18.2 lysoPC.a.C20.3
1           37.9           2.66          0.446           9.00           8.58           7.27           1.83
4           32.8           2.39          0.323           7.21           7.22           7.62           1.64
5           24.5           1.27          0.382           6.66           5.39           3.60           0.97
8           33.7           3.09          0.455           6.96           7.31           7.53           2.35
9           36.0           3.46          0.435           7.27           8.11           6.75           2.08
  lysoPC.a.C20.4 lysoPC.a.C24.0 lysoPC.a.C26.0 lysoPC.a.C26.1 lysoPC.a.C28.0 lysoPC.a.C28.1 PC.aa.C24.0
1          8.25          0.079          0.113          0.053          0.108          0.072       0.082
4          6.75          0.066          0.086          0.045          0.076          0.076       0.076
5          6.26          0.084          0.118          0.053          0.092          0.072       0.069
8          8.73          0.061          0.083          0.047          0.124          0.078       0.082
9          7.82          0.068          0.083          0.037          0.096          0.061       0.064
  PC.aa.C26.0 PC.aa.C28.1 PC.aa.C30.0 PC.aa.C32.0 PC.aa.C32.1 PC.aa.C32.2 PC.aa.C32.3 PC.aa.C34.1 PC.aa.C34.2
1       0.438       0.571        2.35        11.4        9.22          NA       0.092       109.0        71.0
4       0.486       0.685        3.33        18.6       13.30       0.053       0.079       106.0        93.6
5       0.401       0.513        1.78        13.8        5.03          NA       0.102        83.4        35.9
8       0.424       0.605        2.32        12.1       11.50          NA       0.093        83.6        60.6
9       0.430       0.486        2.05        10.4       11.40          NA       0.082        89.6        55.1
  PC.aa.C34.3 PC.aa.C34.4 PC.aa.C36.0 PC.aa.C36.1 PC.aa.C36.2 PC.aa.C36.3 PC.aa.C36.4 PC.aa.C36.5 PC.aa.C36.6
1       1.430       0.200        2.38        21.7        42.4        42.7       120.0        1.86       0.084
4       1.590       0.190        2.57        20.9        48.8        41.2       122.0        1.76       0.070
5       0.709       0.135        1.83        20.5        28.5        21.9        98.1        1.70       0.048
8       1.580       0.251        2.16        18.4        34.4        41.5       110.0        2.03       0.106
9       1.390       0.221        1.62        18.3        32.0        41.8       102.0        1.77       0.081
  PC.aa.C38.0 PC.aa.C38.3 PC.aa.C38.4 PC.aa.C38.5 PC.aa.C38.6 PC.aa.C40.1 PC.aa.C40.2 PC.aa.C40.3 PC.aa.C40.4
1       1.230        32.1        95.1        16.8        41.6       0.195       0.074       0.491        3.48
4       1.160        28.7        92.7        14.3        29.9       0.220       0.097       0.433        3.59
5       1.100        23.3       101.0        13.8        36.2       0.165       0.044       0.525        3.37
```

```
8       1.150        31.3        81.7        14.5        42.8       0.225       0.099       0.384        4.02
9       0.902        31.1        75.9        13.6        37.6       0.181       0.100       0.298        2.88
  PC.aa.C40.5 PC.aa.C40.6 PC.aa.C42.0 PC.aa.C42.1 PC.aa.C42.2 PC.aa.C42.4 PC.aa.C42.5 PC.aa.C42.6 PC.ae.C30.0
1        5.66        21.8       0.364       0.226       0.108       0.272       0.272       0.291       0.173
4        5.06        14.0       0.427       0.223       0.119       0.268       0.267       0.254       0.223
5        5.29        22.5       0.125       0.095       0.083       0.206       0.205       0.280       0.095
8        5.49        20.6       0.365       0.193       0.089       0.266       0.237       0.288       0.212
9        4.88        17.5       0.396       0.216       0.086       0.215       0.206       0.223       0.179
  PC.ae.C30.1 PC.ae.C30.2 PC.ae.C32.1 PC.ae.C32.2 PC.ae.C34.0 PC.ae.C34.1 PC.ae.C34.2 PC.ae.C34.3 PC.ae.C36.0
1       0.027       0.022        1.65       0.371       0.880        3.66        2.48       0.813       0.498
4       0.049       0.023        2.47       0.459       0.964        4.06        3.09       1.020       0.552
5       0.082       0.023        1.72       0.316       1.060        3.28        1.70       0.722       0.553
8       0.028       0.033        1.68       0.335       1.140        3.51        2.28       0.868       0.479
9       0.012       0.022        1.53       0.291       0.683        3.20        2.03       0.663       0.384
  PC.ae.C36.1 PC.ae.C36.2 PC.ae.C36.3 PC.ae.C36.4 PC.ae.C36.5 PC.ae.C38.0 PC.ae.C38.1 PC.ae.C38.2 PC.ae.C38.3
1        5.64        1.90        1.17        6.96        4.79       0.474       0.287       0.538        2.66
4        4.75        2.01        1.35        8.36        5.97       0.397       0.022       0.144        1.97
5        5.95        1.47        0.76        4.78        4.00       0.430       0.271       0.246        1.80
8        5.65        1.97        1.25        7.15        4.04       0.550       0.078       0.559        2.90
9        4.79        1.54        1.12        6.43        3.32       0.442          NA       0.224        2.53
  PC.ae.C38.4 PC.ae.C38.5 PC.ae.C38.6 PC.ae.C40.1 PC.ae.C40.2 PC.ae.C40.3 PC.ae.C40.4 PC.ae.C40.5 PC.ae.C40.6
1        6.33        5.51        1.95       0.574       0.575       0.940        1.76        1.77        1.59
4        5.99        5.63        1.97       0.425       0.540       0.742        1.45        1.62        1.25
5        5.45        4.34        1.51       0.430       0.432       0.632        1.10        1.25        1.47
8        5.73        4.53        1.71       0.584       0.499       0.991        1.84        1.53        1.46
9        5.03        3.82        1.28       0.472       0.555       0.737        1.35        1.34        1.21
  PC.ae.C42.0 PC.ae.C42.1 PC.ae.C42.2 PC.ae.C42.3 PC.ae.C42.4 PC.ae.C42.5 PC.ae.C44.3 PC.ae.C44.4 PC.ae.C44.5
1       0.629       0.316       0.192       0.277       0.264       0.888       0.065       0.168       0.536
4       0.637       0.299       0.159       0.208       0.392       0.863       0.069       0.237       0.517
5       0.660       0.355       0.138       0.174       0.162       0.513       0.081       0.154       0.178
8       0.631       0.271       0.186       0.282       0.333       0.861       0.085       0.183       0.534
9       0.645       0.264       0.168       0.229       0.319       0.925       0.069       0.184       0.671
  PC.ae.C44.6 SM..OH..C14.1 SM..OH..C16.1 SM..OH..C22.1 SM..OH..C22.2 SM..OH..C24.1 SM.C16.0 SM.C16.1 SM.C18.0
1       0.494         1.420         1.330          2.07          1.86         0.597     44.9     7.99     14.5
4       0.611         1.720         1.480          2.97          2.84         0.682     52.4     8.61     17.2
5       0.134         0.987         1.480          1.96          1.74         0.478     40.6     5.86     13.0
8       0.429         1.500         1.160          2.98          2.59         0.631     37.9     7.92     11.9
9       0.460         1.230         0.984          2.21          2.07         0.507     37.3     6.65     12.0
  SM.C18.1 SM.C20.2 SM.C24.0 SM.C24.1 SM.C26.0 SM.C26.1 H1_1   H1 Urea_N L.Arginine_N L.Leucine_N EDTAca_N
1    10.40    0.290    12.20     27.3    0.147    0.337 3356 3356     NA          NA          NA       NA
4    11.50    0.261    11.80     27.9    0.138    0.353 2652 2652  500.8        16.0        27.1      2.5
5     8.34    0.196     9.29     20.5    0.111    0.283 2258 2258  132.5        13.2        57.9      2.5
8     9.59    0.199     9.36     18.8    0.117    0.227 2464 2464  182.3        49.8        63.9      0.0
9     8.48    0.183    10.30     23.6    0.090    0.268 2725 2725  255.8        39.0        64.6      2.7
  X2.Hydroxybutyrate X3.Hydroxybutyrate Acetate Acetoacetate Acetone Betaine Carnitine Choline Creatine
1                 NA                 NA      NA           NA      NA      NA        NA      NA       NA
4               12.7                7.2     9.8          4.8     4.0    13.9       7.7    11.8     14.7
5               35.2               44.7    20.2         18.9    18.9    33.9      18.5    27.7     35.4
8               21.7               20.9    19.5         15.4     6.6    35.3      13.0    21.5     25.9
9               17.1               37.9    20.0         22.0     9.3    12.0      14.4    15.4     25.3
  Dimethyl.sulfone Ethanol Formate Glucose Glycerol Hypoxanthine Isobutyrate Isopropanol Lactate Malonate
1               NA      NA      NA      NA       NA           NA          NA          NA      NA       NA
4              1.3     6.4    14.4   629.5    322.0          8.6         2.5         4.4  1037.7      7.6
5              5.5    13.0    40.0  1618.0    271.6          0.0         6.1        11.2  2199.9     11.7
8              5.4    10.2    23.2  2120.5    406.5          5.8         4.5         4.4  1661.4     11.0
9              3.5     5.1    25.0  1644.2    479.9          5.6         5.9         6.7  2048.5      8.0
 [ reached 'max' / getOption("max.print") -- omitted 1 rows ]
```

d. Median **c4-OH-Pro** value if missing

```
> mb2 <- median(mb1$c4.OH.Pro, na.rm = TRUE)
> mb1$c4.OH.Pro[is.na(mb1$c4.OH.Pro)] <- mb2
> head(mb1)
     Label  Phe Pro Ser Thr ADMA alpha.AAA c4.OH.Pro Carnosine Creatinine  DOPA Dopamine Histamine Kynurenine
1 Alzheimer 72.8 166 170 282 1.15     0.760     0.236     1.270       49.9 0.265    0.233     0.225       5.21
4 Alzheimer 94.1 129 162 201 1.10     0.795     0.199     0.675       80.1 0.264    0.234     0.209       5.80
5 Alzheimer 79.8 126 115 199 1.24     1.360     0.199     1.280       60.5 0.271    0.231     0.210       4.46
8   Healthy 83.6 119 135 268 1.18     0.779     0.215     0.647       30.6 0.275    0.244     0.214       5.66
9   Healthy 73.7 124 145 307 1.17     0.785     0.186     0.590       39.8 0.259    0.233     0.210       6.36
```

	Met.SO	Nitro.Tyr	PEA	Putrescine	Sarcosine	Serotonin	Spermidine	Spermine	t4.OH.Pro	Taurine	SDMA	C0	C10
1	0.526	0.027	NA	0.068	17.8	0.147	0.188	NA	24.0	125	1.13	18.2	0.059
4	0.389	NA	NA	0.110	18.7	0.255	0.353	NA	23.1	159	1.34	23.5	0.071
5	0.466	NA	NA	0.118	22.5	0.390	0.473	NA	26.9	149	1.24	13.6	0.139
8	0.245	0.002	NA	0.161	23.3	0.215	0.276	NA	10.7	133	1.04	13.3	0.051
9	0.413	NA	NA	0.121	22.1	0.166	0.327	NA	16.0	215	1.24	15.8	0.061

	C10.1	C10.2	C12	C12.DC	C12.1	C14	C14.1	C14.1.OH	C14.2	C14.2.OH	C16	C16.OH	C16.1	C16.1.OH	C16.2
1	0.312	0.038	0.030	0.042	0.290	0.023	0.019	0.008	0.008	0.006	0.046	0.008	0.009	0.007	0.005
4	0.317	0.040	0.045	0.048	0.275	0.026	0.028	0.010	0.013	0.011	0.074	0.011	0.015	0.008	0.006
5	0.472	0.074	0.056	0.079	0.394	0.034	0.043	0.016	0.025	0.017	0.062	NA	0.024	0.014	0.012
8	0.217	0.030	0.041	0.035	0.174	0.024	0.017	0.007	0.006	0.007	0.060	0.006	0.010	0.005	0.004
9	0.258	0.036	0.037	0.038	0.228	0.022	0.018	0.007	0.007	0.007	0.054	0.005	0.012	0.005	0.005

	C16.2.OH	C18	C18.1	C18.1.OH	C18.2	C2	C3	C3.OH	C3.1	C4	C3.DC..C4.OH.	C4.1	C5	C5.M.DC
1	0.013	0.013	0.024	0.003	0.016	1.97	0.354	0.008	0.015	0.082	0.045	0.025	0.094	0.023
4	0.009	0.020	0.035	0.004	0.033	2.10	0.278	0.010	0.017	0.110	0.077	0.031	0.145	0.034
5	0.025	0.031	0.034	0.012	0.017	5.62	0.436	0.029	0.035	0.106	0.099	0.069	0.141	0.094
8	0.008	0.020	0.025	0.004	0.019	1.66	0.258	0.008	0.012	0.082	0.047	0.021	0.107	0.023
9	0.009	0.014	0.026	0.003	0.016	2.21	0.233	0.008	0.014	0.088	0.029	0.024	0.127	0.024

	C5.OH..C3.DC.M.	C5.1	C5.1.DC	C6..C4.1.DC.	C5.DC..C6.OH.	C6.1	C7.DC	C8	C9	lysoPC.a.C14.0
1	0.026	0.030	0.020	0.022	0.014	0.018	0.011	0.062	0.016	2.23
4	0.041	0.035	0.016	0.029	0.016	0.027	0.017	0.091	0.018	2.19
5	0.058	0.073	0.049	0.052	0.040	0.040	0.036	0.192	0.041	1.88
8	0.023	0.021	0.017	0.036	0.011	NA	0.009	0.062	0.011	2.13
9	0.024	0.025	0.016	0.026	0.018	0.015	0.013	0.064	0.014	2.10

	lysoPC.a.C16.0	lysoPC.a.C16.1	lysoPC.a.C17.0	lysoPC.a.C18.0	lysoPC.a.C18.1	lysoPC.a.C18.2	lysoPC.a.C20.3
1	37.9	2.66	0.446	9.00	8.58	7.27	1.83
4	32.8	2.39	0.323	7.21	7.22	7.62	1.64
5	24.5	1.27	0.382	6.66	5.39	3.60	0.97
8	33.7	3.09	0.455	6.96	7.31	7.53	2.35
9	36.0	3.46	0.435	7.27	8.11	6.75	2.08

	lysoPC.a.C20.4	lysoPC.a.C24.0	lysoPC.a.C26.0	lysoPC.a.C26.1	lysoPC.a.C28.0	lysoPC.a.C28.1	PC.aa.C24.0
1	8.25	0.079	0.113	0.053	0.108	0.072	0.082
4	6.75	0.066	0.086	0.045	0.076	0.076	0.076
5	6.26	0.084	0.118	0.053	0.092	0.072	0.069
8	8.73	0.061	0.083	0.047	0.124	0.078	0.082
9	7.82	0.068	0.083	0.037	0.096	0.061	0.064

	PC.aa.C26.0	PC.aa.C28.1	PC.aa.C30.0	PC.aa.C32.0	PC.aa.C32.1	PC.aa.C32.2	PC.aa.C32.3	PC.aa.C34.1	PC.aa.C34.2
1	0.438	0.571	2.35	11.4	9.22	NA	0.092	109.0	71.0
4	0.486	0.685	3.33	18.6	13.30	0.053	0.079	106.0	93.6
5	0.401	0.513	1.78	13.8	5.03	NA	0.102	83.4	35.9
8	0.424	0.605	2.32	12.1	11.50	NA	0.093	83.6	60.6
9	0.430	0.486	2.05	10.4	11.40	NA	0.082	89.6	55.1

	PC.aa.C34.3	PC.aa.C34.4	PC.aa.C36.0	PC.aa.C36.1	PC.aa.C36.2	PC.aa.C36.3	PC.aa.C36.4	PC.aa.C36.5	PC.aa.C36.6
1	1.430	0.200	2.38	21.7	42.4	42.7	120.0	1.86	0.084
4	1.590	0.190	2.57	20.9	48.8	41.2	122.0	1.76	0.070
5	0.709	0.135	1.83	20.5	28.5	21.9	98.1	1.70	0.048
8	1.580	0.251	2.16	18.4	34.4	41.5	110.0	2.03	0.106
9	1.390	0.221	1.62	18.3	32.0	41.8	102.0	1.77	0.081

	PC.aa.C38.0	PC.aa.C38.3	PC.aa.C38.4	PC.aa.C38.5	PC.aa.C38.6	PC.aa.C40.1	PC.aa.C40.2	PC.aa.C40.3	PC.aa.C40.4
1	1.230	32.1	95.1	16.8	41.6	0.195	0.074	0.491	3.48
4	1.160	28.7	92.7	14.3	29.9	0.220	0.097	0.433	3.59
5	1.100	23.3	101.0	13.8	36.2	0.165	0.044	0.525	3.37
8	1.150	31.3	81.7	14.5	42.8	0.225	0.099	0.384	4.02
9	0.902	31.1	75.9	13.6	37.6	0.181	0.100	0.298	2.88

	PC.aa.C40.5	PC.aa.C40.6	PC.aa.C42.0	PC.aa.C42.1	PC.aa.C42.2	PC.aa.C42.4	PC.aa.C42.5	PC.aa.C42.6	PC.ae.C30.0
1	5.66	21.8	0.364	0.226	0.108	0.272	0.272	0.291	0.173
4	5.06	14.0	0.427	0.223	0.119	0.268	0.267	0.254	0.223
5	5.29	22.5	0.125	0.095	0.083	0.206	0.205	0.280	0.095
8	5.49	20.6	0.365	0.193	0.089	0.266	0.237	0.288	0.212
9	4.88	17.5	0.396	0.216	0.086	0.215	0.206	0.223	0.179

	PC.ae.C30.1	PC.ae.C30.2	PC.ae.C32.1	PC.ae.C32.2	PC.ae.C34.0	PC.ae.C34.1	PC.ae.C34.2	PC.ae.C34.3	PC.ae.C36.0
1	0.027	0.022	1.65	0.371	0.880	3.66	2.48	0.813	0.498
4	0.049	0.023	2.47	0.459	0.964	4.06	3.09	1.020	0.552
5	0.082	0.023	1.72	0.316	1.060	3.28	1.70	0.722	0.553
8	0.028	0.033	1.68	0.335	1.140	3.51	2.28	0.868	0.479
9	0.012	0.022	1.53	0.291	0.683	3.20	2.03	0.663	0.384

	PC.ae.C36.1	PC.ae.C36.2	PC.ae.C36.3	PC.ae.C36.4	PC.ae.C36.5	PC.ae.C38.0	PC.ae.C38.1	PC.ae.C38.2	PC.ae.C38.3
1	5.64	1.90	1.17	6.96	4.79	0.474	0.287	0.538	2.66
4	4.75	2.01	1.35	8.36	5.97	0.397	0.022	0.144	1.97
5	5.95	1.47	0.76	4.78	4.00	0.430	0.271	0.246	1.80
8	5.65	1.97	1.25	7.15	4.04	0.550	0.078	0.559	2.90

```
9        4.79        1.54        1.12        6.43        3.32       0.442          NA       0.224        2.53
  PC.ae.C38.4 PC.ae.C38.5 PC.ae.C38.6 PC.ae.C40.1 PC.ae.C40.2 PC.ae.C40.3 PC.ae.C40.4 PC.ae.C40.5 PC.ae.C40.6
1        6.33        5.51        1.95       0.574       0.575       0.940        1.76        1.77        1.59
4        5.99        5.63        1.97       0.425       0.540       0.742        1.45        1.62        1.25
5        5.45        4.34        1.51       0.430       0.432       0.632        1.10        1.25        1.47
8        5.73        4.53        1.71       0.584       0.499       0.991        1.84        1.53        1.46
9        5.03        3.82        1.28       0.472       0.555       0.737        1.35        1.34        1.21
  PC.ae.C42.0 PC.ae.C42.1 PC.ae.C42.2 PC.ae.C42.3 PC.ae.C42.4 PC.ae.C42.5 PC.ae.C44.3 PC.ae.C44.4 PC.ae.C44.5
1       0.629       0.316       0.192       0.277       0.264       0.888       0.065       0.168       0.536
4       0.637       0.299       0.159       0.208       0.392       0.863       0.069       0.237       0.517
5       0.660       0.355       0.138       0.174       0.162       0.513       0.081       0.154       0.178
8       0.631       0.271       0.186       0.282       0.333       0.861       0.085       0.183       0.534
9       0.645       0.264       0.168       0.229       0.319       0.925       0.069       0.184       0.671
  PC.ae.C44.6 SM..OH..C14.1 SM..OH..C16.1 SM..OH..C22.1 SM..OH..C22.2 SM..OH..C24.1 SM.C16.0 SM.C16.1 SM.C18.0
1       0.494         1.420         1.330          2.07          1.86         0.597     44.9     7.99     14.5
4       0.611         1.720         1.480          2.97          2.84         0.682     52.4     8.61     17.2
5       0.134         0.987         1.480          1.96          1.74         0.478     40.6     5.86     13.0
8       0.429         1.500         1.160          2.98          2.59         0.631     37.9     7.92     11.9
9       0.460         1.230         0.984          2.21          2.07         0.507     37.3     6.65     12.0
  SM.C18.1 SM.C20.2 SM.C24.0 SM.C24.1 SM.C26.0 SM.C26.1 H1_1   H1 Urea_N L.Arginine_N L.Leucine_N EDTAca_N
1    10.40    0.290    12.20     27.3    0.147    0.337 3356 3356     NA           NA          NA       NA
4    11.50    0.261    11.80     27.9    0.138    0.353 2652 2652  500.8         16.0        27.1      2.5
5     8.34    0.196     9.29     20.5    0.111    0.283 2258 2258  132.5         13.2        57.9      2.5
8     9.59    0.199     9.36     18.8    0.117    0.227 2464 2464  182.3         49.8        63.9      0.0
9     8.48    0.183    10.30     23.6    0.090    0.268 2725 2725  255.8         39.0        64.6      2.7
  X2.Hydroxybutyrate X3.Hydroxybutyrate Acetate Acetoacetate Acetone Betaine Carnitine Choline Creatine
1                 NA                 NA      NA           NA      NA      NA        NA      NA       NA
4               12.7                7.2     9.8          4.8     4.0    13.9       7.7    11.8     14.7
5               35.2               44.7    20.2         18.9    18.9    33.9      18.5    27.7     35.4
8               21.7               20.9    19.5         15.4     6.6    35.3      13.0    21.5     25.9
9               17.1               37.9    20.0         22.0     9.3    12.0      14.4    15.4     25.3
  Dimethyl.sulfone Ethanol Formate Glucose Glycerol Hypoxanthine Isobutyrate Isopropanol Lactate Malonate
1               NA      NA      NA      NA       NA           NA          NA          NA      NA       NA
4              1.3     6.4    14.4   629.5    322.0          8.6         2.5         4.4  1037.7      7.6
5              5.5    13.0    40.0  1618.0    271.6          0.0         6.1        11.2  2199.9     11.7
8              5.4    10.2    23.2  2120.5    406.5          5.8         4.5         4.4  1661.4     11.0
9              3.5     5.1    25.0  1644.2    479.9          5.6         5.9         6.7  2048.5      8.0
 [ reached 'max' / getOption("max.print") -- omitted 1 rows ]
```

e. Drop columns with > 25% missing values

```
> mb3 <- colSums(is.na(mb1)) <= 0.25 * nrow(mb1)
> head(mb1 <- mb1[, mb3])
     Label  Phe Pro Ser Thr ADMA alpha.AAA c4.OH.Pro Carnosine Creatinine  DOPA Dopamine Histamine Kynurenine
1 Alzheimer 72.8 166 170 282 1.15     0.760     0.236     1.270       49.9 0.265    0.233     0.225       5.21
4 Alzheimer 94.1 129 162 201 1.10     0.795     0.199     0.675       80.1 0.264    0.234     0.209       5.80
5 Alzheimer 79.8 126 115 199 1.24     1.360     0.199     1.280       60.5 0.271    0.231     0.210       4.46
8   Healthy 83.6 119 135 268 1.18     0.779     0.215     0.647       30.6 0.275    0.244     0.214       5.66
9   Healthy 73.7 124 145 307 1.17     0.785     0.186     0.590       39.8 0.259    0.233     0.210       6.36
  Met.SO Putrescine Sarcosine Serotonin Spermidine t4.OH.Pro Taurine SDMA   C0   C10 C10.1 C10.2   C12 C12.DC
1  0.526      0.068      17.8     0.147      0.188      24.0     125 1.13 18.2 0.059 0.312 0.038 0.030  0.042
4  0.389      0.110      18.7     0.255      0.353      23.1     159 1.34 23.5 0.071 0.317 0.040 0.045  0.048
5  0.466      0.118      22.5     0.390      0.473      26.9     149 1.24 13.6 0.139 0.472 0.074 0.056  0.079
8  0.245      0.161      23.3     0.215      0.276      10.7     133 1.04 13.3 0.051 0.217 0.030 0.041  0.035
9  0.413      0.121      22.1     0.166      0.327      16.0     215 1.24 15.8 0.061 0.258 0.036 0.037  0.038
  C12.1   C14 C14.1 C14.1.OH C14.2 C14.2.OH   C16 C16.OH C16.1 C16.1.OH C16.2 C16.2.OH   C18 C18.1 C18.1.OH
1 0.290 0.023 0.019    0.008 0.008    0.006 0.046  0.008 0.009    0.007 0.005    0.013 0.013 0.024    0.003
4 0.275 0.026 0.028    0.010 0.013    0.011 0.074  0.011 0.015    0.008 0.006    0.009 0.020 0.035    0.004
5 0.394 0.034 0.043    0.016 0.025    0.017 0.062     NA 0.024    0.014 0.012    0.025 0.031 0.034    0.012
8 0.174 0.024 0.017    0.007 0.006    0.007 0.060  0.006 0.010    0.005 0.004    0.008 0.020 0.025    0.004
9 0.228 0.022 0.018    0.007 0.007    0.007 0.054  0.005 0.012    0.005 0.005    0.009 0.014 0.026    0.003
  C18.2   C2    C3 C3.OH  C3.1    C4 C3.DC..C4.OH.  C4.1    C5 C5.M.DC C5.OH..C3.DC.M.  C5.1 C5.1.DC
1 0.016 1.97 0.354 0.008 0.015 0.082         0.045 0.025 0.094   0.023           0.026 0.030   0.020
4 0.033 2.10 0.278 0.010 0.017 0.110         0.077 0.031 0.145   0.034           0.041 0.035   0.016
5 0.017 5.62 0.436 0.029 0.035 0.106         0.099 0.069 0.141   0.094           0.058 0.073   0.049
8 0.019 1.66 0.258 0.008 0.012 0.082         0.047 0.021 0.107   0.023           0.023 0.021   0.017
9 0.016 2.21 0.233 0.008 0.014 0.088         0.029 0.024 0.127   0.024           0.024 0.025   0.016
  C6..C4.1.DC. C5.DC..C6.OH.  C6.1 C7.DC    C8    C9 lysoPC.a.C14.0 lysoPC.a.C16.0 lysoPC.a.C16.1
1        0.022         0.014 0.018 0.011 0.062 0.016           2.23           37.9           2.66
4        0.029         0.016 0.027 0.017 0.091 0.018           2.19           32.8           2.39
```

5	0.052	0.040	0.040	0.036	0.192	0.041	1.88	24.5	1.27	
8	0.036	0.011	NA	0.009	0.062	0.011	2.13	33.7	3.09	
9	0.026	0.018	0.015	0.013	0.064	0.014	2.10	36.0	3.46	

	lysoPC.a.C17.0	lysoPC.a.C18.0	lysoPC.a.C18.1	lysoPC.a.C18.2	lysoPC.a.C20.3	lysoPC.a.C20.4	lysoPC.a.C24.0
1	0.446	9.00	8.58	7.27	1.83	8.25	0.079
4	0.323	7.21	7.22	7.62	1.64	6.75	0.066
5	0.382	6.66	5.39	3.60	0.97	6.26	0.084
8	0.455	6.96	7.31	7.53	2.35	8.73	0.061
9	0.435	7.27	8.11	6.75	2.08	7.82	0.068

	lysoPC.a.C26.0	lysoPC.a.C26.1	lysoPC.a.C28.0	lysoPC.a.C28.1	PC.aa.C24.0	PC.aa.C26.0	PC.aa.C28.1	PC.aa.C30.0
1	0.113	0.053	0.108	0.072	0.082	0.438	0.571	2.35
4	0.086	0.045	0.076	0.076	0.076	0.486	0.685	3.33
5	0.118	0.053	0.092	0.072	0.069	0.401	0.513	1.78
8	0.083	0.047	0.124	0.078	0.082	0.424	0.605	2.32
9	0.083	0.037	0.096	0.061	0.064	0.430	0.486	2.05

	PC.aa.C32.0	PC.aa.C32.1	PC.aa.C32.3	PC.aa.C34.1	PC.aa.C34.2	PC.aa.C34.3	PC.aa.C34.4	PC.aa.C36.0	PC.aa.C36.1
1	11.4	9.22	0.092	109.0	71.0	1.430	0.200	2.38	21.7
4	18.6	13.30	0.079	106.0	93.6	1.590	0.190	2.57	20.9
5	13.8	5.03	0.102	83.4	35.9	0.709	0.135	1.83	20.5
8	12.1	11.50	0.093	83.6	60.6	1.580	0.251	2.16	18.4
9	10.4	11.40	0.082	89.6	55.1	1.390	0.221	1.62	18.3

	PC.aa.C36.2	PC.aa.C36.3	PC.aa.C36.4	PC.aa.C36.5	PC.aa.C36.6	PC.aa.C38.0	PC.aa.C38.3	PC.aa.C38.4	PC.aa.C38.5
1	42.4	42.7	120.0	1.86	0.084	1.230	32.1	95.1	16.8
4	48.8	41.2	122.0	1.76	0.070	1.160	28.7	92.7	14.3
5	28.5	21.9	98.1	1.70	0.048	1.100	23.3	101.0	13.8
8	34.4	41.5	110.0	2.03	0.106	1.150	31.3	81.7	14.5
9	32.0	41.8	102.0	1.77	0.081	0.902	31.1	75.9	13.6

	PC.aa.C38.6	PC.aa.C40.1	PC.aa.C40.2	PC.aa.C40.3	PC.aa.C40.4	PC.aa.C40.5	PC.aa.C40.6	PC.aa.C42.0	PC.aa.C42.1
1	41.6	0.195	0.074	0.491	3.48	5.66	21.8	0.364	0.226
4	29.9	0.220	0.097	0.433	3.59	5.06	14.0	0.427	0.223
5	36.2	0.165	0.044	0.525	3.37	5.29	22.5	0.125	0.095
8	42.8	0.225	0.099	0.384	4.02	5.49	20.6	0.365	0.193
9	37.6	0.181	0.100	0.298	2.88	4.88	17.5	0.396	0.216

	PC.aa.C42.2	PC.aa.C42.4	PC.aa.C42.5	PC.aa.C42.6	PC.ae.C30.0	PC.ae.C30.1	PC.ae.C30.2	PC.ae.C32.1	PC.ae.C32.2
1	0.108	0.272	0.272	0.291	0.173	0.027	0.022	1.65	0.371
4	0.119	0.268	0.267	0.254	0.223	0.049	0.023	2.47	0.459
5	0.083	0.206	0.205	0.280	0.095	0.082	0.023	1.72	0.316
8	0.089	0.266	0.237	0.288	0.212	0.028	0.033	1.68	0.335
9	0.086	0.215	0.206	0.223	0.179	0.012	0.022	1.53	0.291

	PC.ae.C34.0	PC.ae.C34.1	PC.ae.C34.2	PC.ae.C34.3	PC.ae.C36.0	PC.ae.C36.1	PC.ae.C36.2	PC.ae.C36.3	PC.ae.C36.4
1	0.880	3.66	2.48	0.813	0.498	5.64	1.90	1.17	6.96
4	0.964	4.06	3.09	1.020	0.552	4.75	2.01	1.35	8.36
5	1.060	3.28	1.70	0.722	0.553	5.95	1.47	0.76	4.78
8	1.140	3.51	2.28	0.868	0.479	5.65	1.97	1.25	7.15
9	0.683	3.20	2.03	0.663	0.384	4.79	1.54	1.12	6.43

	PC.ae.C36.5	PC.ae.C38.0	PC.ae.C38.2	PC.ae.C38.3	PC.ae.C38.4	PC.ae.C38.5	PC.ae.C38.6	PC.ae.C40.1	PC.ae.C40.2
1	4.79	0.474	0.538	2.66	6.33	5.51	1.95	0.574	0.575
4	5.97	0.397	0.144	1.97	5.99	5.63	1.97	0.425	0.540
5	4.00	0.430	0.246	1.80	5.45	4.34	1.51	0.430	0.432
8	4.04	0.550	0.559	2.90	5.73	4.53	1.71	0.584	0.499
9	3.32	0.442	0.224	2.53	5.03	3.82	1.28	0.472	0.555

	PC.ae.C40.3	PC.ae.C40.4	PC.ae.C40.5	PC.ae.C40.6	PC.ae.C42.0	PC.ae.C42.1	PC.ae.C42.2	PC.ae.C42.3	PC.ae.C42.4
1	0.940	1.76	1.77	1.59	0.629	0.316	0.192	0.277	0.264
4	0.742	1.45	1.62	1.25	0.637	0.299	0.159	0.208	0.392
5	0.632	1.10	1.25	1.47	0.660	0.355	0.138	0.174	0.162
8	0.991	1.84	1.53	1.46	0.631	0.271	0.186	0.282	0.333
9	0.737	1.35	1.34	1.21	0.645	0.264	0.168	0.229	0.319

	PC.ae.C42.5	PC.ae.C44.3	PC.ae.C44.4	PC.ae.C44.5	PC.ae.C44.6	SM..OH..C14.1	SM..OH..C16.1	SM..OH..C22.1
1	0.888	0.065	0.168	0.536	0.494	1.420	1.330	2.07
4	0.863	0.069	0.237	0.517	0.611	1.720	1.480	2.97
5	0.513	0.081	0.154	0.178	0.134	0.987	1.480	1.96
8	0.861	0.085	0.183	0.534	0.429	1.500	1.160	2.98
9	0.925	0.069	0.184	0.671	0.460	1.230	0.984	2.21

	SM..OH..C22.2	SM..OH..C24.1	SM.C16.0	SM.C16.1	SM.C18.0	SM.C18.1	SM.C20.2	SM.C24.0	SM.C24.1	SM.C26.0	SM.C26.1
1	1.86	0.597	44.9	7.99	14.5	10.40	0.290	12.20	27.3	0.147	0.337
4	2.84	0.682	52.4	8.61	17.2	11.50	0.261	11.80	27.9	0.138	0.353
5	1.74	0.478	40.6	5.86	13.0	8.34	0.196	9.29	20.5	0.111	0.283
8	2.59	0.631	37.9	7.92	11.9	9.59	0.199	9.36	18.8	0.117	0.227
9	2.07	0.507	37.3	6.65	12.0	8.48	0.183	10.30	23.6	0.090	0.268

	H1_1	H1	Urea_N	L.Arginine_N	L.Leucine_N	EDTAca_N	X2.Hydroxybutyrate	X3.Hydroxybutyrate	Acetate	
1	3356	3356	NA	NA	NA	NA	NA	NA	NA	

```
4 2652 2652  500.8         16.0        27.1      2.5              12.7               7.2     9.8
5 2258 2258  132.5         13.2        57.9      2.5              35.2              44.7    20.2
8 2464 2464  182.3         49.8        63.9      0.0              21.7              20.9    19.5
9 2725 2725  255.8         39.0        64.6      2.7              17.1              37.9    20.0
  Acetoacetate Acetone Betaine Carnitine Choline Creatine Dimethyl.sulfone Ethanol Formate Glucose Glycerol
1           NA      NA      NA        NA      NA       NA               NA      NA      NA      NA       NA
4          4.8     4.0    13.9       7.7    11.8     14.7              1.3     6.4    14.4   629.5    322.0
5         18.9    18.9    33.9      18.5    27.7     35.4              5.5    13.0    40.0  1618.0    271.6
8         15.4     6.6    35.3      13.0    21.5     25.9              5.4    10.2    23.2  2120.5    406.5
9         22.0     9.3    12.0      14.4    15.4     25.3              3.5     5.1    25.0  1644.2    479.9
  Hypoxanthine Isobutyrate Isopropanol Lactate Malonate
1           NA          NA          NA      NA       NA
4          8.6         2.5         4.4  1037.7      7.6
5          0.0         6.1        11.2  2199.9     11.7
8          5.8         4.5         4.4  1661.4     11.0
9          5.6         5.9         6.7  2048.5      8.0
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